



3 March 2000

Chemical Physics Letters 318 (2000) 662–672

**CHEMICAL  
PHYSICS  
LETTERS**

www.elsevier.nl/locate/cplett

## Author index to Volume 318

- Abbott, J., see Castle, K.J. 318 (2000) 565
- Abu-Eittah, R.H., H. Moustafa and A.M. Al-Omar, The electronic structure of some acyl azides: cyclic–open tautomerism 318 (2000) 276
- Aguilar, A., see Aquilanti, V. 318 (2000) 619
- Aguirre, F., J. Husband, C.J. Thompson and R.B. Metz, Gas-phase photodissociation of  $\text{AuCH}_2^+$ : the dissociation threshold of jet-cooled and rotationally thermalized ions 318 (2000) 466
- Akiyama, Y., see Nakano, T. 318 (2000) 614
- Akutsu, H., see Saito, K. 318 (2000) 75
- Al-Omar, A.M., see Abu-Eittah, R.H. 318 (2000) 276
- Amiot, C., J. Vergès, J. d'Incan and C. Effantin, Corrigendum to: “The  $(3)^1\Pi-(3)^1\Sigma^+$  systems of  $\text{KRb}$ ” [Chem. Phys. Lett. 315 (1999) 55–60] 318 (2000) 289
- Anderson, L.W., see Peck, J.R. 318 (2000) 476
- Andrés, J., see Castillo, R. 318 (2000) 270
- Andrés, J., see Safont, V.S. 318 (2000) 361
- Andrianov, I., V. Bonačić-Koutecký, M. Hartmann, J. Manz, J. Pittner and K. Sundermann, Ab initio three-dimensional quantum dynamics of  $\text{Ag}_3$  clusters in the NeNePo process 318 (2000) 256
- Aquilanti, V., G. Capecchi, S. Cavalli, D. De Fazio, P. Palmieri, C. Puzzarini, A. Aguilar, X. Giménez and J.M. Lucas, The  $\text{He} + \text{H}_2^+$  reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern 318 (2000) 619
- Ariga, K., see Furukawa, K. 318 (2000) 22
- Aristov, V., D. Conroy and H. Reisler, Symmetry and lifetime of the hydroxymethyl radical in the 3p Rydberg state 318 (2000) 393
- Au, F.C.K., see Zhou, X.T. 318 (2000) 58
- Balasubramanian, K., see Feng, P.Y. 318 (2000) 417
- Baldwin, L.C., see Sulkes, M. 318 (2000) 448
- Barisien, T., see Pham, T.-A. 318 (2000) 459
- Bauer, E., see Schmidt, Th. 318 (2000) 549
- Bello, I., see Zhou, X.T. 318 (2000) 58
- Bezerra Jr., A.G., I.E. Borissevitch, R.E. de Araujo, A.S.L. Gomes and C.B. de Araújo, Investigation of picosecond optical nonlinearity in porphyrin metal complexes derivatives 318 (2000) 511
- Bigot, J.-Y., see Pham, T.-A. 318 (2000) 459
- Bludský, O., P. Nachtigall, J. Hrušák and P. Jensen, The calculation of the vibrational states of  $\text{SO}_2$  in the  $\tilde{\text{C}}^1\text{B}_2$  electronic state up to the  $\text{SO}(^3\Sigma^-) + \text{O}(^3\text{P})$  dissociation limit 318 (2000) 607
- Blyth, R.I.R., see Duschek, R. 318 (2000) 43

- Boens, N., see Molski, A. 318 (2000) 325
- Boillot, M.L., see Bousseksou, A. 318 (2000) 409
- Bojarski, P., L. Kuřak and J. Kubicki, Donor fluorescence decay in the presence of forward and reverse excitation energy transport in two-component disordered systems 318 (2000) 379
- Bonaćić-Koutecký, V., see Andrianov, I. 318 (2000) 256
- Borissevitch, I.E., see Bezerra Jr., A.G. 318 (2000) 511
- Bousseksou, A., J.J. McGarvey, F. Varret, J.A. Real, J.-P. Tuchagues, A.C. Dennis and M.L. Boillot, Raman spectroscopy of the high- and low-spin states of the spin crossover complex  $\text{Fe}(\text{phen})_2(\text{NCS})_2$ : an initial approach to estimation of vibrational contributions to the associated entropy change 318 (2000) 409
- Bruna, P.J. and F. Grein, Theoretical study of the electron-spin magnetic moment (*g*-tensor) of  $\text{FCI}^-$  318 (2000) 263
- Buchachenko, A.A., T. González-Lezana, M.I. Hernández, M.P. de Lara Castells, G. Delgado-Barrio and P. Villarreal, Blueshifts of the  $\text{B} \leftarrow \text{X}$  excitation spectra of  $\text{He}^{79}\text{Br}_2$  using a DIM-based potential 318 (2000) 578
- Bunker, P.R., see Osmann, G. 318 (2000) 597
- Caleyo, F., see Venegas, V. 318 (2000) 655
- Capecchi, G., see Aquilanti, V. 318 (2000) 619
- Castillo, R., V. Moliner and J. Andrés, A theoretical study on the molecular mechanism for the normal Reimer-Tiemann reaction 318 (2000) 270
- Castle, K.J., J. Abbott, X. Peng and W. Kong, Photodissociation of *t*-butyl nitrite between 220 and 250 nm: internal energy distribution of NO 318 (2000) 565
- Castleman Jr., A.W., see Folmer, D.E. 318 (2000) 637
- Catalán, J., J.C. del Valle and M. Kasha, Conformity of the 7-azaindole dimer cationic potential with photoionization/Coulomb-explosion MS observations and the concerted biprotonic transfer mechanism 318 (2000) 629
- Cavalli, S., see Aquilanti, V. 318 (2000) 619
- Chan, S.P., see Liu, Z.F. 318 (2000) 15
- Chandra, A.K., T. Uchimaru, M. Sugie and A. Sekiya, Correlation between hardness and activation energies for reactions of OH radical with halomethanes 318 (2000) 69
- Chaplin, M.F., see Du, Z. 318 (2000) 319
- Chen, H.M., see Chen, X.L. 318 (2000) 107
- Chen, X.L., H.M. Chen, J. Li, Y.M. Liu, X.C. Dai, G.H. Sha, J.C. Xie, C.H. Zhang and L. Li, Quantum interference effect on collisional energy transfer within singlet ~ triplet mixed states of  $\text{Na}_2$   $\text{A}^1\Sigma_u^+(v=8) \sim \text{b}^3\Pi_{0u}(v=14)$  318 (2000) 107
- Chen, Y., see Palmer, P.M. 318 (2000) 440
- Chin, B.-C., K. Misawa, T. Masuda and T. Kobayashi, Large static dipole moment in substituted polyacetylenes obtained by electroabsorption 318 (2000) 499
- Civalleri, B., see Ugliengo, P. 318 (2000) 247
- Cocchi, M., see Giro, G. 318 (2000) 137
- Conroy, D., see Aristov, V. 318 (2000) 393
- Couris, S., see Konstantaki, M. 318 (2000) 488
- Coxon, J.A., see Melville, T.C. 318 (2000) 454
- Cumings, J. and A. Zettl, Erratum to: "Mass-production of boron nitride double-wall nanotubes and nanococoons" [Chem. Phys. Lett. 316 (2000) 211-216] 318 (2000) 497

- Dai, X.C., see Chen, X.L. 318 (2000) 107
- De Araújo, C.B., see Bezerra Jr., A.G. 318 (2000) 511
- De Araujo, R.E., see Bezerra Jr., A.G. 318 (2000) 511
- Deckert, V., see Stöckle, R.M. 318 (2000) 131
- De Fazio, D., see Aquilanti, V. 318 (2000) 619
- De Lara Castells, M.P., see Buchachenko, A.A. 318 (2000) 578
- Delgado-Barrio, G., see Buchachenko, A.A. 318 (2000) 578
- Del Valle, J.C., see Catalán, J. 318 (2000) 629
- Dennis, A.C., see Bousseksou, A. 318 (2000) 409
- Deratani, A., see Konstantaki, M. 318 (2000) 488
- De Schryver, F., see Molski, A. 318 (2000) 325
- Dhanya, S., R.D. Saini, P.D. Naik and R.K. Vatsa, Formation of BrO in the photo oxidation of CF<sub>2</sub>Br<sub>2</sub> 318 (2000) 125
- Dierksen, G.H.F., see Yamamoto, S. 318 (2000) 590
- Di Marco, P., see Giro, G. 318 (2000) 137
- D'Incan, J., see Amiot, C. 318 (2000) 289
- Dobkowski, J., V. Galievsky, A. Starukhin and J. Waluk, Relaxation in excited states of porphycene in low-temperature argon and nitrogen matrices 318 (2000) 79
- Dong, X., Z. Guilan, W. Haiyan, T. Guoqing and C. Wenju, Study on dynamic optical nonlinearities of excited state proton transfer in ethanol solution of 7-hydroxyquinoline 318 (2000) 433
- Dovesi, R., see Lichanot, A. 318 (2000) 240
- Dovesi, R., see Ugliengo, P. 318 (2000) 247
- Du, Z., L.J. Dunne, G. Manos and M.F. Chaplin, Exact statistical mechanical treatment of benzene adsorption in a zeolite twin-pore one-dimensional lattice model 318 (2000) 319
- Dunne, L.J., see Du, Z. 318 (2000) 319
- Duschek, R., F. Mittendorfer, R.I.R. Blyth, F.P. Netzer, J. Hafner and M.G. Ramsey, The adsorption of aromatics on sp-metals: benzene on Al(111) 318 (2000) 43
- Dutta-Roy, B., see Gangopadhyay, D. 318 (2000) 161
- Eddaoudi, H., see Konstantaki, M. 318 (2000) 488
- Effantin, C., see Amiot, C. 318 (2000) 289
- El-Nahas, A.M., N. Tajima and K. Hirao, Do Cu<sup>2+</sup>NH<sub>3</sub> and Cu<sup>2+</sup>OH<sub>2</sub> exist?: theory confirms 'yes!' 318 (2000) 333
- Ervin, K.M., see Shi, Y. 318 (2000) 149
- Fang, W.-H., see Liu, D. 318 (2000) 291
- Fattori, V., see Giro, G. 318 (2000) 137
- Feng, P.Y. and K. Balasubramanian, Potential energy surfaces of electronic states of AlP<sub>2</sub>, Al<sub>2</sub>P and their ions 318 (2000) 417
- Fichou, D., see Knupfer, M. 318 (2000) 585
- Fink, J., see Knupfer, M. 318 (2000) 585
- Fink, M.J., see Sulkes, M. 318 (2000) 448
- Finley, J.P., Diagrammatic CASPT2 using an internally contracted basis 318 (2000) 190
- Fleniken, J., Y. Kim and H. Meyer, Efficient production of vibrationally excited NO using a pulsed molecular beam discharge source 318 (2000) 529
- Fleniken, J., see Kim, Y. 318 (2000) 522
- Folmer, D.E., E.S. Wisniewski and A.W. Castleman Jr., Excited state double proton transfer in the 7-azaindole dimer revisited 318 (2000) 637



- Fu, X.-Y., see Liu, D. 318 (2000) 291
- Fu, Z., see Zhou, M. 318 (2000) 644
- Furukawa, K., S.R. Tian, H. Yamauchi, S. Yamazaki, H. Ijiri, K. Ariga and K. Muraoka, Characterization of H-Y zeolite modified by a radio-frequency CF<sub>4</sub> plasma 318 (2000) 22
- Galievsky, V., see Dobkowski, J. 318 (2000) 79
- Gangopadhyay, D., B.N. Ganguly, T. Mukherjee and B. Dutta-Roy, Anti-Arrhenius behaviour in positronium chemistry: a Kramers' turnover? 318 (2000) 161
- Ganguly, B.N., see Gangopadhyay, D. 318 (2000) 161
- Gawandi, V.B., H. Mohan and J.P. Mittal, Erratum to: "Role of solute structure on the stability of the OH-adduct of substituted organic sulfides and its transformation to a radical cation". [Chem. Phys. Lett. 314 (1999) 451-458] 318 (2000) 496
- Geetha, B. and A.B. Mandal, 2-Dimensional surface properties of  $\omega$ -methoxy poly(ethylene glycol) macromonomer and homopolymer at the air-water interface 318 (2000) 35
- Gensch, T., see Molski, A. 318 (2000) 325
- Giménez, X., see Aquilanti, V. 318 (2000) 619
- Giro, G., M. Cocchi, J. Kalinowski, P. Di Marco and V. Fattori, Multicomponent emission from organic light emitting diodes based on polymer dispersion of an aromatic diamine and an oxadiazole derivative 318 (2000) 137
- Gödicke, B., A. Langenscheidt, H. Meyer and A. Schweig, Formation of persistent contact ion pairs in solid argon 318 (2000) 102
- Goh, S.H., see Jin, Z. 318 (2000) 505
- Gomes, A.S.L., see Bezerra Jr., A.G. 318 (2000) 511
- González-Lezana, T., see Buchachenko, A.A. 318 (2000) 578
- Grayer, V., see Pham, T.-A. 318 (2000) 459
- Grein, F., see Bruna, P.J. 318 (2000) 263
- Guidoni, L., see Pham, T.-A. 318 (2000) 459
- Guilan, Z., see Dong, X. 318 (2000) 433
- Günther, S., see Schmidt, Th. 318 (2000) 549
- Guo, L., Z. Wu, T. Liu, W. Wang and H. Zhu, Synthesis of novel Sb<sub>2</sub>O<sub>3</sub> and Sb<sub>2</sub>O<sub>5</sub> nanorods 318 (2000) 49
- Guoqing, T., see Dong, X. 318 (2000) 433
- Hadziioannou, G., see Pham, T.-A. 318 (2000) 459
- Hafner, J., see Duschek, R. 318 (2000) 43
- Haiyan, W., see Dong, X. 318 (2000) 433
- Han, S.Y., see Kim, S.Y. 318 (2000) 63
- Hara, K., see Ito, N. 318 (2000) 118
- Harata, A., see Ito, K. 318 (2000) 1
- Hartmann, M., see Andrianov, I. 318 (2000) 256
- Hernández, E., see Seifert, G. 318 (2000) 355
- Hernández, M.I., see Buchachenko, A.A. 318 (2000) 578
- Hirao, K., see El-Nahas, A.M. 318 (2000) 333
- Ho, M.-S., see Sun, Y.-C. 318 (2000) 7
- Hofkens, J., see Molski, A. 318 (2000) 325
- Horimoto, N., J.-y. Kohno, F. Mafuné and T. Kondow, Ejection mechanism of molecules and neutral clusters from liquid beam under irradiation of IR laser 318 (2000) 536
- Houston, P.L., see Pisano, P.J. 318 (2000) 385

- Hrušák, J., see Bludský, O. 318 (2000) 607  
Huang, T.-H., see Wei, T.-H. 318 (2000) 53  
Husband, J., see Aguirre, F. 318 (2000) 466
- Ijiri, H., see Furukawa, K. 318 (2000) 22  
Ikeda, T., T. Kodaira, F. Izumi, T. Kamiyama and K. Ohshima, Neutron powder diffraction study of potassium clusters in zeolite K-LTA 318 (2000) 93  
Imbihl, R., see Schmidt, Th. 318 (2000) 549  
Ito, F. and T. Nakanaga, A jet-cooled infrared spectrum of the formic acid dimer by cavity ring-down spectroscopy 318 (2000) 571  
Ito, K., I. Tsuyumoto, A. Harata and T. Sawada, Ultrafast energy transfer of silver ultrafine particles in aqueous solutions as investigated by the ultrafast lensing effect technique 318 (2000) 1  
Ito, N., O. Kajimoto and K. Hara, Picosecond time-resolved fluorescence depolarization of *p*-terphenyl at high pressures 318 (2000) 118  
Iwataki, T., see Mayama, H. 318 (2000) 113  
Izumi, F., see Ikeda, T. 318 (2000) 93
- Jackson, B., see Shalashilin, D.V. 318 (2000) 305  
Janot, J.M., see Konstantaki, M. 318 (2000) 488  
Jedlovsky, P., M. Mezei and R. Vallauri, A molecular level explanation of the density maximum of liquid water from computer simulations with a polarizable potential model 318 (2000) 155  
Jensen, P., see Osmann, G. 318 (2000) 597  
Jensen, P., see Bludský, O. 318 (2000) 607  
Ji, W., see Jin, Z. 318 (2000) 505  
Jin, Z., X. Sun, G. Xu, S.H. Goh and W. Ji, Nonlinear optical properties of some polymer/multi-walled carbon nanotube composites 318 (2000) 505  
Jouguelet, E., C. Mathis and P. Petit, Controlling the electronic properties of single-wall carbon nanotubes by chemical doping 318 (2000) 561
- Kajimoto, O., see Ito, N. 318 (2000) 118  
Kalinowski, J., see Giro, G. 318 (2000) 137  
Kaminuma, T., see Nakano, T. 318 (2000) 614  
Kamiyama, T., see Ikeda, T. 318 (2000) 93  
Karelson, M., see Yamamoto, S. 318 (2000) 590  
Kasha, M., see Catalán, J. 318 (2000) 629  
Katrusiak, A., see Szafranski, M. 318 (2000) 427  
Kawahara, S., see Uchimaru, T. 318 (2000) 203  
Kawai, A., R. Kohno, N. Oki and K. Obi, Exciplex formation reaction in benzaldehyde-1,4-dimethoxybenzene clusters 318 (2000) 85  
Kawamura, Y., see Nakai, H. 318 (2000) 298  
Kellö, V., P. Pyykkö, A.J. Sadlej, P. Schwerdtfeger and J. Thyssen, The nuclear quadrupole moment of <sup>91</sup>Zr from molecular data for ZrO and ZrS 318 (2000) 222  
Kharlanov, V., see Rettig, W. 318 (2000) 173  
Kim, J., see Vijaya Sarathy, K. 318 (2000) 543  
Kim, S.Y., G.Y. Lee, S.Y. Han and M. Lee, Fluorescence quenching dynamics of azulene and 2-haloazulenes by CCl<sub>4</sub> in nonpolar solvents 318 (2000) 63  
Kim, Y., K. Patton, J. Fleniken and H. Meyer, Rotationally resolved overtone spectroscopy of the NO-Ar complex 318 (2000) 522

- Kim, Y., see Fleniken, J. 318 (2000) 529
- Kitaura, K., see Nakano, T. 318 (2000) 614
- Knupfer, M., J. Fink, E. Zojer, G. Leising and D. Fichou, Universal exciton size scaling in  $\pi$  conjugated systems 318 (2000) 585
- Kobayashi, T., see Chin, B.-C. 318 (2000) 499
- Kodaira, T., see Ikeda, T. 318 (2000) 93
- Kohno, J.-y., see Horimoto, N. 318 (2000) 536
- Kohno, R., see Kawai, A. 318 (2000) 85
- Kondow, T., see Horimoto, N. 318 (2000) 536
- Kong, W., see Castle, K.J. 318 (2000) 565
- Konstantaki, M., E. Koudoumas, S. Couris, J.M. Janot, H. Eddaoudi, A. Deratani, P. Seta and S. Leach, Optical limiting behaviour of the water-soluble  $C_{60}/\gamma$ -cyclodextrin complex 318 (2000) 488
- Korchowiec, J., see Uchimaru, T. 318 (2000) 203
- Koudoumas, E., see Konstantaki, M. 318 (2000) 488
- Kraemer, W.P., see Osmann, G. 318 (2000) 597
- Kruger, C.H., see Zhao, M. 318 (2000) 555
- Kryachko, E.S., Generalized idempotency purification transform in linear scaling self-consistent field theory 318 (2000) 210
- Kubicki, J., see Bojarski, P. 318 (2000) 379
- Kulak, L., see Bojarski, P. 318 (2000) 379
- Kuo, C.T., see Nee, J.B. 318 (2000) 402
- Lai, H.L., see Zhou, X.T. 318 (2000) 58
- Lai, M.Y., see Mebel, A.M. 318 (2000) 27
- Langenscheidt, A., see Gödicke, B. 318 (2000) 102
- Largent, C.C., see Zhao, M. 318 (2000) 555
- Lawler, J.E., see Peck, J.R. 318 (2000) 476
- Leach, S., see Konstantaki, M. 318 (2000) 488
- Lee, C.S., see Zhou, X.T. 318 (2000) 58
- Lee, E.P.F. and T.G. Wright,  $NO^+ \cdot O_2$  versus  $NO_3^+$  – which is the more stable? 318 (2000) 196
- Lee, G.Y., see Kim, S.Y. 318 (2000) 63
- Lee, M., see Kim, S.Y. 318 (2000) 63
- Lee, S.T., see Zhou, X.T. 318 (2000) 58
- Leising, G., see Knupfer, M. 318 (2000) 585
- Li, J., see Chen, X.L. 318 (2000) 107
- Li, L., see Chen, X.L. 318 (2000) 107
- Liao, L.S., see Zhou, X.T. 318 (2000) 58
- Lichanot, A., R. Orlando, G. Mallia, M. Mérawa and R. Dovesi,  $V_{OH}$  center in magnesium oxide: an ab initio supercell study 318 (2000) 240
- Lin, M.-S., see Wei, T.-H. 318 (2000) 53
- Liu, D., W.-H. Fang and X.-Y. Fu, Ab initio molecular orbital study of the mechanism of photodissociation of formamide 318 (2000) 291
- Liu, T., see Guo, L. 318 (2000) 49
- Liu, Y.M., see Chen, X.L. 318 (2000) 107
- Liu, Z.F. and S.P. Chan, Dissociative chemisorption of molecular chlorine on Si(100) – a first principles study 318 (2000) 15



- Lu, H.-F., see Sun, Y.-C. 318 (2000) 7
- Lucas, J.M., see Aquilanti, V. 318 (2000) 619
- Mafuné, F., see Horimoto, N. 318 (2000) 536
- Mallia, G., see Lichanot, A. 318 (2000) 240
- Mandal, A.B., see Geetha, B. 318 (2000) 35
- Manos, G., see Du, Z. 318 (2000) 319
- Manz, J., see Andrianov, I. 318 (2000) 256
- Marcus, R.K. and R.W. Schwartz, Compositional profiling of solution-deposited lead zirconate–titanate thin films by radio-frequency glow discharge atomic emission spectroscopy (rf-GD-AES) 318 (2000) 481
- Maroulis, G., Is the dipole polarizability of hydrogen iodide accurately known? 318 (2000) 181
- Masuda, T., see Chin, B.-C. 318 (2000) 499
- Mathis, C., see Jouguelet, E. 318 (2000) 561
- Matsumura, K., see Uchimaru, T. 318 (2000) 203
- Maus, M., see Rettig, W. 318 (2000) 173
- Mayama, H., T. Iwataki and K. Yoshikawa, Thermodynamics in the folding phase-transition of single T4DNA molecules in poly(ethylene glycol) solution 318 (2000) 113
- McGarvey, J.J., see Bousseksou, A. 318 (2000) 409
- Mebel, A.M., M.Y. Lai and Y.L. Wang, Two-dimensional Ga-induced magic clusters on the Si surface: a density functional study 318 (2000) 27
- Melville, T.C. and J.A. Coxon, The first spectroscopic observation of YbS: the  $A0^+ - X0^+$  visible laser excitation spectrum 318 (2000) 454
- Mérawa, M., see Lichanot, A. 318 (2000) 240
- Metz, R.B., see Aguirre, F. 318 (2000) 466
- Meyer, H., see Gödicke, B. 318 (2000) 102
- Meyer, H., see Kim, Y. 318 (2000) 522
- Meyer, H., see Fleniken, J. 318 (2000) 529
- Mezei, M., see Jedlovsky, P. 318 (2000) 155
- Misawa, K., see Chin, B.-C. 318 (2000) 499
- Mittal, J.P., see Gawandi, V.B. 318 (2000) 496
- Mittendorfer, F., see Duschek, R. 318 (2000) 43
- Mohan, H., see Gawandi, V.B. 318 (2000) 496
- Moliner, V., see Castillo, R. 318 (2000) 270
- Molski, A., J. Hofkens, T. Gensch, N. Boens and F. De Schryver, Theory of time-resolved single-molecule fluorescence spectroscopy 318 (2000) 325
- Mota, F., see Novoa, J.J. 318 (2000) 345
- Moustafa, H., see Abu-Eittah, R.H. 318 (2000) 276
- Mukherjee, T., see Gangopadhyay, D. 318 (2000) 161
- Muraoka, K., see Furukawa, K. 318 (2000) 22
- Myszkiewicz, G. and J. Sadlej, Ab initio study for the intermolecular potential of the water–nitric oxide complex 318 (2000) 232
- Nachtigall, P., see Bludský, O. 318 (2000) 607
- Naik, P.D., see Dhanya, S. 318 (2000) 125
- Nakai, H. and Y. Kawamura,  $\pi$ – $\sigma$  Hyperconjugation mechanism on the rotational barrier of the methyl group (II): 1- and 2-methylnaphthalenes in the  $S_0$ ,  $S_1$ ,  $C_0$ , and  $A_1$  states 318 (2000) 298
- Nakanaga, T., see Ito, F. 318 (2000) 571

- Nakano, T., T. Kaminuma, T. Sato, Y. Akiyama, M. Uebayasi and K. Kitaura, Fragment molecular orbital method: application to polypeptides 318 (2000) 614
- Narayan, K.S., see Vijaya Sarathy, K. 318 (2000) 543
- Nee, J.B., C.T. Kuo, H.C. Tseng and S.Y. Wang, Potential energy curves of Xe<sub>2</sub> derived from the pressure-dependent fluorescence excitation spectra of the 1st and 2nd continuum 318 (2000) 402
- Netzer, F.P., see Duschek, R. 318 (2000) 43
- Novoa, J.J. and F. Mota, The C-H ··· π bonds: strength, identification, and hydrogen-bonded nature: a theoretical study 318 (2000) 345
- Obi, K., see Kawai, A. 318 (2000) 85
- Ohshima, K., see Ikeda, T. 318 (2000) 93
- Ohtake, T., N. Sonoyama and T. Sakata, Electrochemical luminescence of ZnGa<sub>2</sub>O<sub>4</sub> semiconductor electrodes activated with Cr and Co 318 (2000) 517
- Okada, M., see Saito, K. 318 (2000) 75
- Oki, N., see Kawai, A. 318 (2000) 85
- Oliva, M., see Safont, V.S. 318 (2000) 361
- Orlando, R., see Lichanot, A. 318 (2000) 240
- Ornellas, F.R., see Resende, S.M. 318 (2000) 340
- Ortiz-López, J., see Venegas, V. 318 (2000) 655
- Osmann, G., P.R. Bunker, W.P. Kraemer and P. Jensen, Coulomb explosion imaging: the CH<sub>2</sub><sup>+</sup>, H<sub>2</sub>O<sup>+</sup> and NH<sub>2</sub><sup>+</sup> ions as benchmarks 318 (2000) 597
- Owano, T.G., see Zhao, M. 318 (2000) 555
- Palmer, P.M., Y. Chen and M.R. Topp, Simple water clusters of Coumarins 151 and 152A studied by IR-UV double resonance spectroscopy 318 (2000) 440
- Palmieri, P., see Aquilanti, V. 318 (2000) 619
- Pan, D. and D.L. Phillips, Investigation of the effects of substitution position on the radical anions of chlorobiphenyls 318 (2000) 214
- Patton, K., see Kim, Y. 318 (2000) 522
- Peck, J.R., X.L. Peng, L.W. Anderson and J.E. Lawler, Ultraviolet reflection-absorption spectroscopy of C<sub>6</sub>H<sub>6</sub> physisorbed on gold 318 (2000) 476
- Peng, H.Y., see Zhou, X.T. 318 (2000) 58
- Peng, X., see Castle, K.J. 318 (2000) 565
- Peng, X.L., see Peck, J.R. 318 (2000) 476
- Pérez-Jiménez, A.J., see Sancho-García, J.C. 318 (2000) 649
- Petit, P., see Jouguelet, E. 318 (2000) 561
- Pham, T.-A., T. Barisien, V. Grayer, L. Guidoni, G. Hadziioannou and J.-Y. Bigot, Gain dynamics in oriented thin films of an oligo(*para*-phenylene vinylene) 318 (2000) 459
- Phillips, D.L., see Pan, D. 318 (2000) 214
- Pisano, P.J., M.S. Westley and P.L. Houston, The NO vibrational state distribution in the reaction O(<sup>1</sup>D) + N<sub>2</sub>O → 2NO 318 (2000) 385
- Pittner, J., see Andrianov, I. 318 (2000) 256
- Pliego Jr., J.R., Electronic spectra of the CH<sub>3</sub>C=N=CXY(X, Y = H, Cl) nitrile ylides: an ab initio multiconfigurational second-order quasidegenerate perturbation theory study 318 (2000) 142
- Puzzarini, C., see Aquilanti, V. 318 (2000) 619
- Pyykkö, P., see Kellö, V. 318 (2000) 222



- Qin, Q., see Zhou, M. 318 (2000) 644
- Ramsey, M.G., see Duschek, R. 318 (2000) 43
- Real, J.A., see Bousseksou, A. 318 (2000) 409
- Reisler, H., see Aristov, V. 318 (2000) 393
- Resende, S.M. and F.R. Ornellas, Atmospheric reaction between the HS radical and chlorine 318 (2000) 340
- Ressel, B., see Schmidt, Th. 318 (2000) 549
- Rettig, W., V. Kharlanov and M. Maus, Excited-state relaxation properties of ionic and nonionic donor-acceptor biphenyl derivatives 318 (2000) 173
- Rueda-Morales, G., see Venegas, V. 318 (2000) 655
- Sadlej, A.J., see Kellö, V. 318 (2000) 222
- Sadlej, J., see Myszkiewicz, G. 318 (2000) 232
- Safont, V.S., M. Oliva, J. Andrés and O. Tapia, Alternative pathways for the C2-C3 bond cleavage and C2 configuration inversion processes for the Rubisco-catalyzed carboxylation sequence 318 (2000) 361
- Saini, R.D., see Dhanya, S. 318 (2000) 125
- Saito, K., M. Okada, H. Akutsu and M. Sorai, Can the molecule involved in a CT interaction reorient itself in the crystal lattice? Phase transition and glass transition in *trans*-stilbene-TCNQ 318 (2000) 75
- Sakata, T., see Ohtake, T. 318 (2000) 517
- Sancho-García, J.C. and A.J. Pérez-Jiménez, A systematic and accurate study of singlet propynylidene 318 (2000) 649
- Sato, T., see Nakano, T. 318 (2000) 614
- Sawada, T., see Ito, K. 318 (2000) 1
- Schaak, A., see Schmidt, Th. 318 (2000) 549
- Schmidt, Th., A. Schaak, S. Günther, B. Ressel, E. Bauer and R. Imbihl, In situ imaging of structural changes in a chemical wave with low-energy electron microscopy: the system Rh(110)/NO + H<sub>2</sub> 318 (2000) 549
- Schütz, M. and H.-J. Werner, Local perturbative triples correction (T) with linear cost scaling 318 (2000) 370
- Schwartz, R.W., see Marcus, R.K. 318 (2000) 481
- Schweig, A., see Gödicke, B. 318 (2000) 102
- Schwerdtfeger, P., see Kellö, V. 318 (2000) 222
- Schwerdtfeger, P., see Seth, M. 318 (2000) 314
- Seifert, G. and E. Hernández, Theoretical prediction of phosphorus nanotubes 318 (2000) 355
- Sekiya, A., see Chandra, A.K. 318 (2000) 69
- Seta, P., see Konstantaki, M. 318 (2000) 488
- Seth, M. and P. Schwerdtfeger, A comparison of relativistic and electron correlation effects for (111)F, (111)H and (111)Li 318 (2000) 314
- Sha, G.H., see Chen, X.L. 318 (2000) 107
- Shalashilin, D.V. and B. Jackson, Guiding paths and time-dependent basis sets for wavefunction propagation 318 (2000) 305
- Shi, Y. and K.M. Ervin, Gas-phase acidity and C-H bond energy of diacetylene 318 (2000) 149
- Sonoyama, N., see Ohtake, T. 318 (2000) 517
- Sorai, M., see Saito, K. 318 (2000) 75
- Starukhin, A., see Dobkowski, J. 318 (2000) 79

- Stöckle, R.M., Y.D. Suh, V. Deckert and R. Zenobi, Nanoscale chemical analysis by tip-enhanced Raman spectroscopy 318 (2000) 131
- Sugie, M., see Chandra, A.K. 318 (2000) 69
- Suh, Y.D., see Stöckle, R.M. 318 (2000) 131
- Sulkes, M., L.C. Baldwin and M.J. Fink, Molecular beam study of possible CVD intermediates from Group-14 organometallic precursors 318 (2000) 448
- Sun, X., see Jin, Z. 318 (2000) 505
- Sun, Y., see Sun, Z. 318 (2000) 471
- Sun, Y.-C., H.-F. Lu and M.-S. Ho, Molecular dynamics simulation of hydrogen isotope-terminated silicon(111) and (110) surfaces: calculation of vibrational energy relaxation rates of hydrogen isotope stretching modes 318 (2000) 7
- Sun, Z., Y. Sun and X. Wang, Investigation of phases in the carbon films deposited by electrolysis of ethanol liquid phase using Raman scattering 318 (2000) 471
- Sundermann, K., see Andrianov, I. 318 (2000) 256
- Szafrański, M. and A. Katrusiak, Thermodynamic behaviour of bistable  $\text{NH}^+ - \text{N}$  hydrogen bonds in monosalts of 1,4-diazabicyclo[2.2.2]octane 318 (2000) 427
- Tajima, N., see El-Nahas, A.M. 318 (2000) 333
- Tapia, O., see Safont, V.S. 318 (2000) 361
- Thompson, C.J., see Aguirre, F. 318 (2000) 466
- Thyssen, J., see Kellö, V. 318 (2000) 222
- Tian, S.R., see Furukawa, K. 318 (2000) 22
- Topp, M.R., see Palmer, P.M. 318 (2000) 440
- Tsai, P.-C., see Wei, T.-H. 318 (2000) 53
- Tseng, H.C., see Nee, J.B. 318 (2000) 402
- Tsuyumoto, I., see Ito, K. 318 (2000) 1
- Tsuzuki, S., see Uchimaru, T. 318 (2000) 203
- Tuchagues, J.-P., see Bousseksou, A. 318 (2000) 409
- Uchimaru, T., J. Korchowiec, S. Tsuzuki, K. Matsumura and S. Kawahara, Importance of secondary electrostatic interactions in hydrogen-bonding complexes: an investigation using the self-consistent charge and configuration method for subsystems 318 (2000) 203
- Uchimaru, T., see Chandra, A.K. 318 (2000) 69
- Uebayasi, M., see Nakano, T. 318 (2000) 614
- Ugliengo, P., B. Civalieri, C.M. Zicovich-Wilson and R. Dovesi, H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach 318 (2000) 247
- Vallauri, R., see Jedlovszky, P. 318 (2000) 155
- Varret, F., see Bousseksou, A. 318 (2000) 409
- Vatsa, R.K., see Dhanya, S. 318 (2000) 125
- Vaval, N., Molecular properties using bi-orthogonal functional: a de-coupled scheme 318 (2000) 168
- Venegas, V., J. Ortiz-López, G. Rueda-Morales and F. Caleyó, Synthesis and characterization of Hg metal-doped  $\text{C}_{60}$  318 (2000) 655
- Vergès, J., see Amiot, C. 318 (2000) 289
- Vijaya Sarathy, K., K.S. Narayan, J. Kim and J.O. White, Novel fluorescence and morphological structures in gold nanoparticle-polyoctylthiophene based thin films 318 (2000) 543
- Villarreal, P., see Buchachenko, A.A. 318 (2000) 578

- Wahl, E.H., see Zhao, M. 318 (2000) 555  
Waluk, J., see Dobkowski, J. 318 (2000) 79  
Wang, N., see Zhou, X.T. 318 (2000) 58  
Wang, S.Y., see Nee, J.B. 318 (2000) 402  
Wang, W., see Guo, L. 318 (2000) 49  
Wang, X., see Sun, Z. 318 (2000) 471  
Wang, Y.L., see Mebel, A.M. 318 (2000) 27  
Wei, T.-H., T.-H. Huang, T.-T. Wu, P.-C. Tsai and M.-S. Lin, Studies of nonlinear absorption and refraction in  $C_{60}$ /toluene solution 318 (2000) 53  
Wenju, C., see Dong, X. 318 (2000) 433  
Werner, H.-J., see Schütz, M. 318 (2000) 370  
Westley, M.S., see Pisano, P.J. 318 (2000) 385  
White, J.O., see Vijaya Sarathy, K. 318 (2000) 543  
Wisniewski, E.S., see Folmer, D.E. 318 (2000) 637  
Wright, T.G., see Lee, E.P.F. 318 (2000) 196  
Wu, T.-T., see Wei, T.-H. 318 (2000) 53  
Wu, Z., see Guo, L. 318 (2000) 49  
  
Xie, J.C., see Chen, X.L. 318 (2000) 107  
Xu, G., see Jin, Z. 318 (2000) 505  
  
Yamamoto, S., G.H.F. Dierksen and M. Karelson, An ab initio CI study of electronic spectra of substituted free-base porphyrins 318 (2000) 590  
Yamauchi, H., see Furukawa, K. 318 (2000) 22  
Yamazaki, S., see Furukawa, K. 318 (2000) 22  
Yoshikawa, K., see Mayama, H. 318 (2000) 113  
  
Zare, R.N., see Zhao, M. 318 (2000) 555  
Zenobi, R., see Stöckle, R.M. 318 (2000) 131  
Zettl, A., see Cumings, J. 318 (2000) 497  
Zhang, C.H., see Chen, X.L. 318 (2000) 107  
Zhang, L., see Zhou, M. 318 (2000) 644  
Zhao, M., E.H. Wahl, T.G. Owano, C.C. Largent, R.N. Zare and C.H. Kruger, Near-surface reduction of cavity ring-down spectroscopy detection sensitivity 318 (2000) 555  
Zhou, M., Z. Fu, L. Zhang and Q. Qin, Structure and stability of LiOMn molecule generated by laser ablation 318 (2000) 644  
Zhou, X.T., H.L. Lai, H.Y. Peng, F.C.K. Au, L.S. Liao, N. Wang, I. Bello, C.S. Lee and S.T. Lee, Thin  $\beta$ -SiC nanorods and their field emission properties 318 (2000) 58  
Zhu, H., see Guo, L. 318 (2000) 49  
Zicovich-Wilson, C.M., see Ugliengo, P. 318 (2000) 247  
Zojer, E., see Knupfer, M. 318 (2000) 585



